We claim:

1. A crystal comprising:

a) a JNK3 protein or homologue thereof; and

b) an inhibitor that is capable of inducing the Met146 in JNK3 or corresponding methionine in the JNK3 homologue to have a $\chi 1$ angle in the range of -120° to -180° and 45° to 180° upon binding.

2. A crystal comprising:

a) a JNK3 protein or homologue thereof; and

b) an inhibitor selected from the group consisting of N-[4-(5-Methyl-3-phenyl-isoxazol-4-yl)-pyrimidin-2-yl]-acetamide, 2,4-Dioxo-6-phenylamino-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid phenylamide, 2-Pyridin-4-yl-thiazole-4-carboxylic acid(3-trifluoromethyl-phenyl)-amide, 4-[5-(4-Fluoro-phenyl)-4-pyridin-4-yl-1*H*-imidazol-2-yl]-phenol and 2-(2,6-Dichloro-phenyl)-2-[5-(2,4-difluorobenzoyl)-pyridin-2-yl]-acetamide.

3. The crystal of claim 1 or 2 which is capable of diffracting X-rays to at least 3.0 Å.

4. The crystal according to claim 1 or 2, wherein the JNK3 protein or homologue thereof is phosphorylated or unphosphorylated.

5. The crystal according to claim 1 or 2, wherein the JNK3 protein is JNK3α1.

6. The crystal according to claim 1 or 2, wherein the JNK3 protein or JNK3 homologue contains a C-terminal deletion of about 20 amino acid residues.

7. The crystal according to claim 1 or 2, wherein the JNK3 protein has an N-terminal deletion of about 40 amino acid residues.

8. A method of producing a JNK3-inhibitor complex crystal or JNK3 homologue-inhibitor complex crystal, comprising the steps of:

a) producing a composition comprising a crystallization solution and a JNK3 protein or homologue thereof complexed with an inhibitor, wherein the inhibitor is capable of inducing the Met146 in the JNK3 protein or corresponding methionine in the JNK3 homologue to have a $\chi 1$ angle in the range of -120° to -180° and 45° to 180°; and

b) subjecting said composition to devices or conditions which promote crystallization.

9. The method of claim 8, wherein the composition is treated with micro-crystals of JNK3 protein, JNK3 protein complexes or homologues thereof after step a) but prior to step b).

10. A crystalline molecule or molecular complex comprising a binding pocket defined by structure coordinates of a set of amino acid residues which correspond to JNK3 amino acid residues Lys93, Ile124, Leu126, Leu144, Met146 according to Figure 1 or 2, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues

of said molecule or molecular complex and said JNK3 amino acid residues is not greater than about 0.3 Å.

11. A crystalline molecule or molecular complex comprising a binding pocket defined by structure coordinates of a set of amino acid residues which correspond to JNK3 amino acid residues Ile70, Gly71, Ser72, Asn152, Cys154 and Gln155 according to Figure 3, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues of said molecule or molecular complex and said JNK3 amino acid residues is not greater than about 1.0 Å.

12. A crystalline molecule or molecular complex comprising a protein defined by structure coordinates of a set of amino acid residues which correspond to JNK3 amino acid residues set forth in Figure 1, wherein the root mean square deviation of the backbone atoms between said set of amino acid residues of said protein and said JNK3 amino acid residues is not more than about 0.9 Å.

13. A crystalline molecular complex comprising a protein defined by structure coordinates of a set of amino acid residues which are identical to JNK3 amino acid residues set forth in Figure 1, wherein the root mean square deviation between all atoms of said set of amino acid residues of said protein and said JNK3 amino acid residues is not more than about 1.3 Å.

14. A crystalline molecular complex comprising a protein kinase, wherein the protein kinase comprises a methionine residue that corresponds to

Met146 of JNK3, wherein the residue has a χ1 angle in the range of about −120° to -180° and 45° to 180°.

15. The crystalline molecular complex of claim 14, wherein the χ1 angle is in the range of -150° to -180°, the χ2 angle is in the range of -150° to -170°, and the χ3 angle is in the range of 95° to 135°.

16. The crystalline molecular complex of claim 14, wherein the χ1 angle is in the range of 60° to 80°, the χ2 angle is in the range of 155° to 175°, and the χ3 angle is in the range of -45° to -65°.

17. The crystalline molecular complex of claim 14, wherein the χ1 angle is in the range of 135° to 155°, the χ2 angle is in the range of -115° to -135°, and the χ3 angle is in the range of -155° to -175°.

18. The crystalline molecule or molecular complex according to any one of claims 10-17, wherein the molecule or molecular complex is a JNK3 protein or JNK3 protein complex, or homologues thereof.

19. A computer comprising:

(a) a machine-readable data storage medium, comprising a data storage material encoded with machine-readable data, wherein said data defines the binding pocket according to any one of claims 10-11 or the protein according to any one of claims 12-17;

(b) a working memory for storing instructions for processing said machine-readable data;

(c) a central processing unit coupled to said working memory and to said machine-readable data storage medium for processing said machine-

readable data and means for generating three-dimensional structural information of said binding pocket or protein; and

(d) output hardware coupled to said central processing unit for outputting three-dimensional structural information of said binding pocket or protein, or information produced using said three-dimensional structural information of said binding pocket or protein.

20. The computer according to claim 19, wherein said data is produced by homology modeling of at least a portion of the structure coordinates of Figure 1, 2 or 3.

21. The computer according to claim 19, wherein said means for generating three-dimensional structural information is provided by means for generating a three-dimensional graphical representation of said binding pocket or protein.

22. The computer according to claim 19, wherein said output hardware is a display terminal, a printer, CD or DVD recorder, ZIP™ or JAZ™ drive, a disk drive, or other machine-readable data storage device.

23. A method for designing, selecting and/or optimizing a chemical entity that binds to the molecule or molecular complex according to any one of the claims 10-17 comprising the steps of:

(a) providing the structure coordinates of said molecule or molecular complex on a computer comprising the means for generating three-dimensional structural information from said structure coordinates; and

(b) designing, selecting and/or optimizing said chemical entity by performing a fitting operation between said chemical entity and said three-dimensional structural information of said molecule or molecular complex.

24. A method for evaluating the ability of a chemical entity to associate with the molecule or molecular complex according to any one of claims 10-17 comprising the steps of:

(a) employing computational means to perform a fitting operation between the chemical entity and the molecule or molecular complex; and

(b) analyzing the results of said fitting operation to quantitate the association between the chemical entity and the molecule or molecular complex.

25. The method according to claim 24, further comprising generating a three-dimensional graphical representation of the molecule or molecular complex prior to step (a).

26. The method of claim 24, wherein the method is for evaluating the ability of a chemical entity to associate with the binding pocket of the molecule or molecular complex.

27. A method of using a computer for evaluating the ability of a chemical entity to associate with the molecule or molecular complex according to any one of claims 10-17, wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining said binding pocket

or protein and means for generating a three-dimensional graphical representation of the binding pocket or protein, and wherein said method comprises the steps of:

(a) positioning a first chemical entity within all or part of said binding pocket or protein using a graphical three-dimensional representation of the structure of the chemical entity and the binding pocket or protein;

(b) performing a fitting operation between said chemical entity and said binding pocket or protein by employing computational means;

(c) analyzing the results of said fitting operation to quantitate the association between said chemical entity and all or part of the binding pocket or protein; and

(d) outputting said quantitated association to suitable output hardware.

28. The method according to claim 27, further comprising the steps of:

(e) repeating steps (a) through (d) with a second chemical entity; and

(f) selecting at least one of said first or second chemical entity that associates with said all or part of said binding pocket or protein based on said quantitated association of said first or second chemical entity.

29. A method for identifying an agonist or antagonist of a molecule or molecular complex according to any one of claims 10-17 comprising the steps of:

(a) using a three-dimensional structure of the molecule or molecular complex to design or select a chemical entity;

(b) contacting the chemical entity with the molecule or the molecular complex;

(c) monitoring the catalytic activity of the molecule or molecular complex; and

(d) classifying the chemical entity as an agonist or antagonist based on the effect of the chemical entity on the catalytic activity of the molecule or molecular complex.

30. A method of utilizing molecular replacement to obtain a structural model of a molecule or a molecular complex of unknown structure, comprising the steps of:

(a) crystallizing said molecule or molecular complex;

(b) generating an X-ray diffraction pattern from said crystallized molecule or molecular complex;

(c) applying at least a portion of the structure coordinates set forth in Figure 1, 2 or 3 or in a homology model thereof to the X-ray diffraction pattern to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex whose structure is unknown; and

(d) generating a structural model of the molecule or molecular complex from the three-dimensional electron density map.

31. The method according to claim 30, wherein the molecule is a JNK3 protein or homologue thereof.

32. The method according to claim 30, wherein the molecular complex is selected from the group consisting of a JNK3 protein complex and a JNK3 homologue complex.